

A More Automated Approach to Data Collection for Macromolecular Crystallography

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With the advances in structure refinement software that can automatically solve structures and the increasing use of robotics at synchrotron beamlines, high throughput crystallography is becoming much more automated. However, one aspect of the process that still requires a certain level of human intervention is during data collection. Web-Ice (Gonzalez A, Moorhead P, McPhillips SE, Song J, Sharp K, Taylor JR, Adams PD, Sauter NK, and Soltis SM, (2008) *J. Appl. Cryst.* **41**, 176-184), jointly developed at the Stanford Synchrotron Radiation Laboratory and the Lawrence Berkeley National Laboratory, aims to address this issue by providing beamline users with a unified, graphical user interface that couples the low level control of the beamline hardware with the processing software (LABELIT, DISTL, MOSFLM) responsible for converting raw diffraction images into data sets suitable for refinement. Web-Ice can also perform automated crystal screening for selecting the best samples and calculation of the optimal strategy for data collection. Recent developments in Web-Ice include automatic handling of ice rings at varying two theta angles, automatic selection of the appropriate space group, and automatic data integration and scaling. Through Web-Ice, the beamline user can be more efficient at the synchrotron by allowing the software to handle the decision making for data collection in routine cases, while retaining the flexibility for more difficult data sets by providing a more user friendly interface for tweaking various parameters and customization of scripts for the data processing software.

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